Supporting Information

Highly efficient and chemoselective hydrogenation of α, β-unsaturated carbonyls over Pd/N-doped hierarchically porous carbon

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Content

Table S1. Elemental analysis results of N-doped carbon, CN.

Element	C	N	H	O（calculated）
Content (%)	85.7	5.3	3.0	6.0

Table S2. Textural properties of the catalyst supports

Entry	catalyst	Specific surface area (m^2/g)	Porous volume (cm^3/g)	Pore Size (nm)
1	Pd/CN	424	0.89	8.3
2	Pd/Cs	393	0.80	12.9
3	Pd/MgO	25	0.15	16.6
4	Pd/TiO_2[a]	51	0.04	21.3

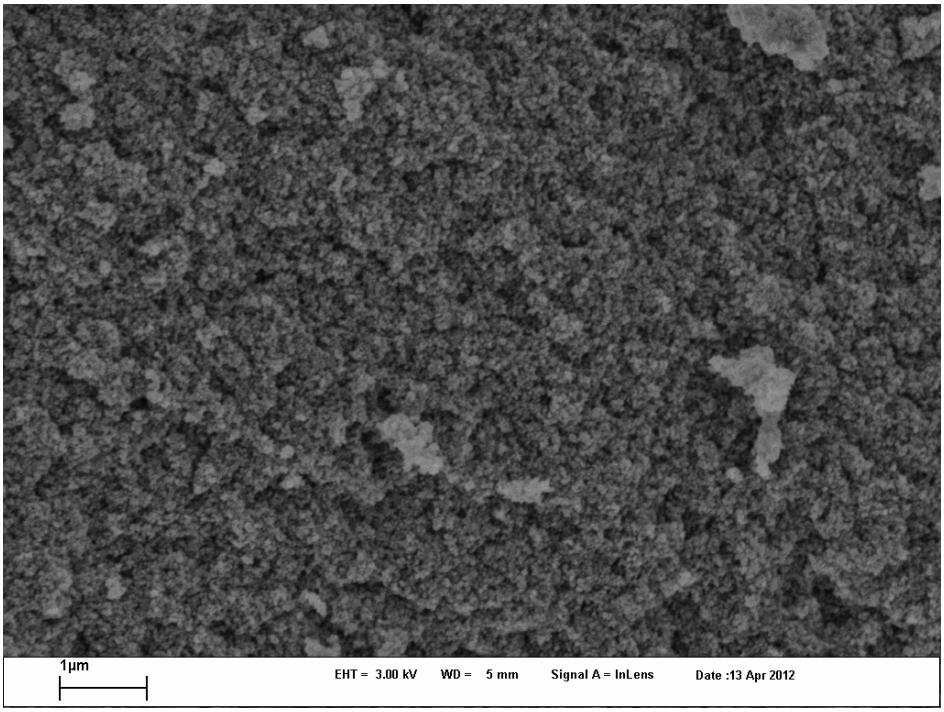
[a]Data from Aladdin Chemistry Co., Ltd.

Table S3. Practical palladium content in the catalysts

catalyst	ICP-AES results	
	fresh	recycle
1.5%Pd/CN	1.476	1.260[a]
1.5%Pd/Cs	1.291	0.815[b]

[a] The Pd content in Pd/CN after 8 times recyles.
[b] The Pd content in Pd/Cs after 3 times recyles.

Figure S1. SEM images of the N-doped carbon materials CN.



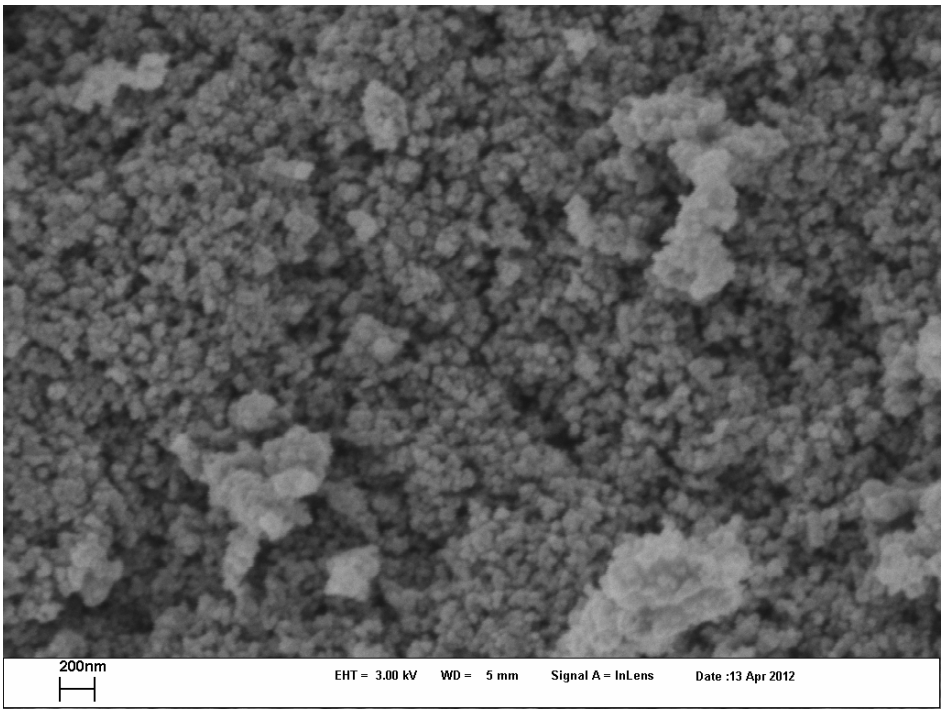
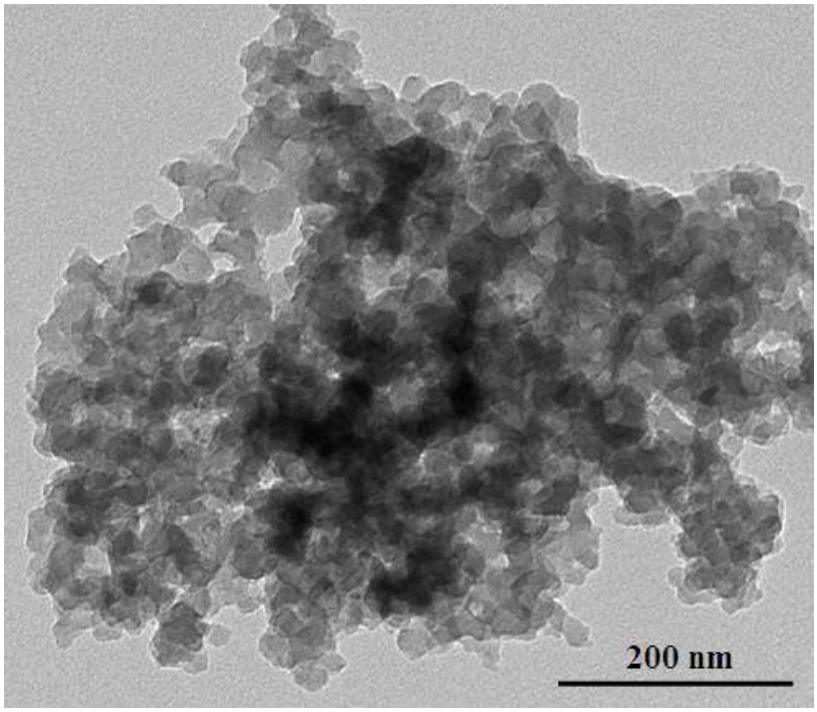


Figure S2. TEM images of Cs.



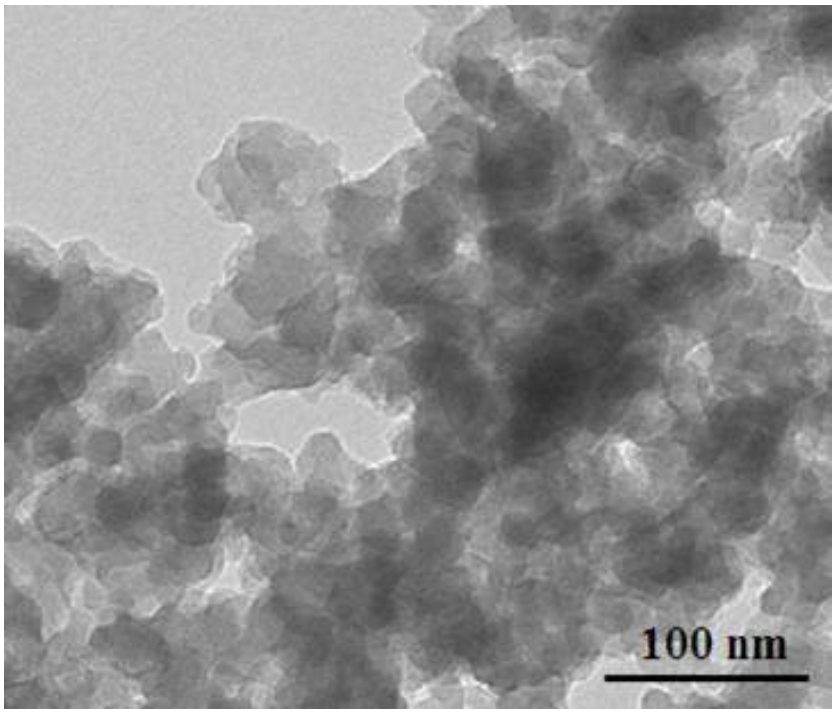


Figure S3: Pore size distributions of CN using DFT model.

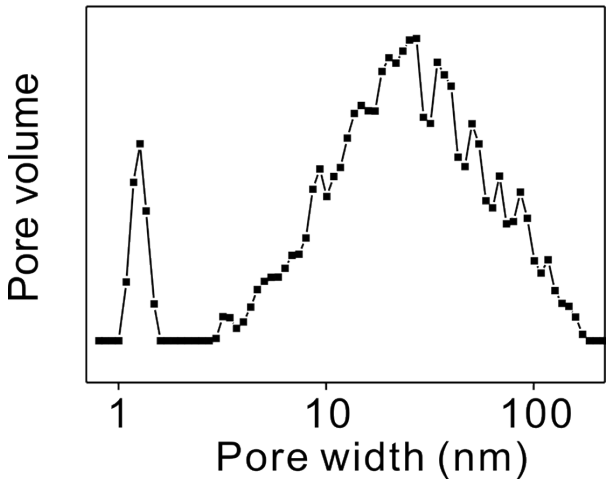


Figure S4: The time-activity profile under different temperatures (conversion below 45%)

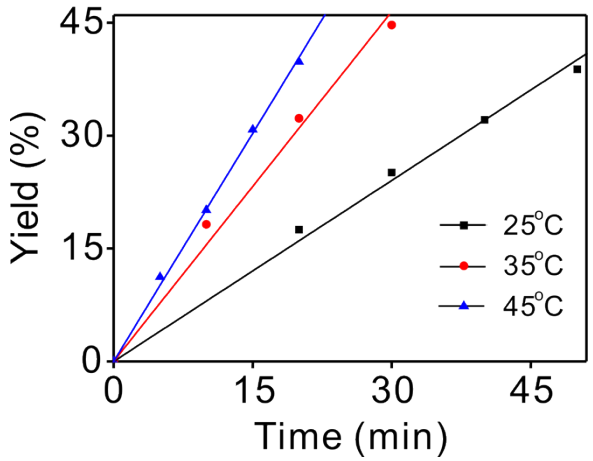
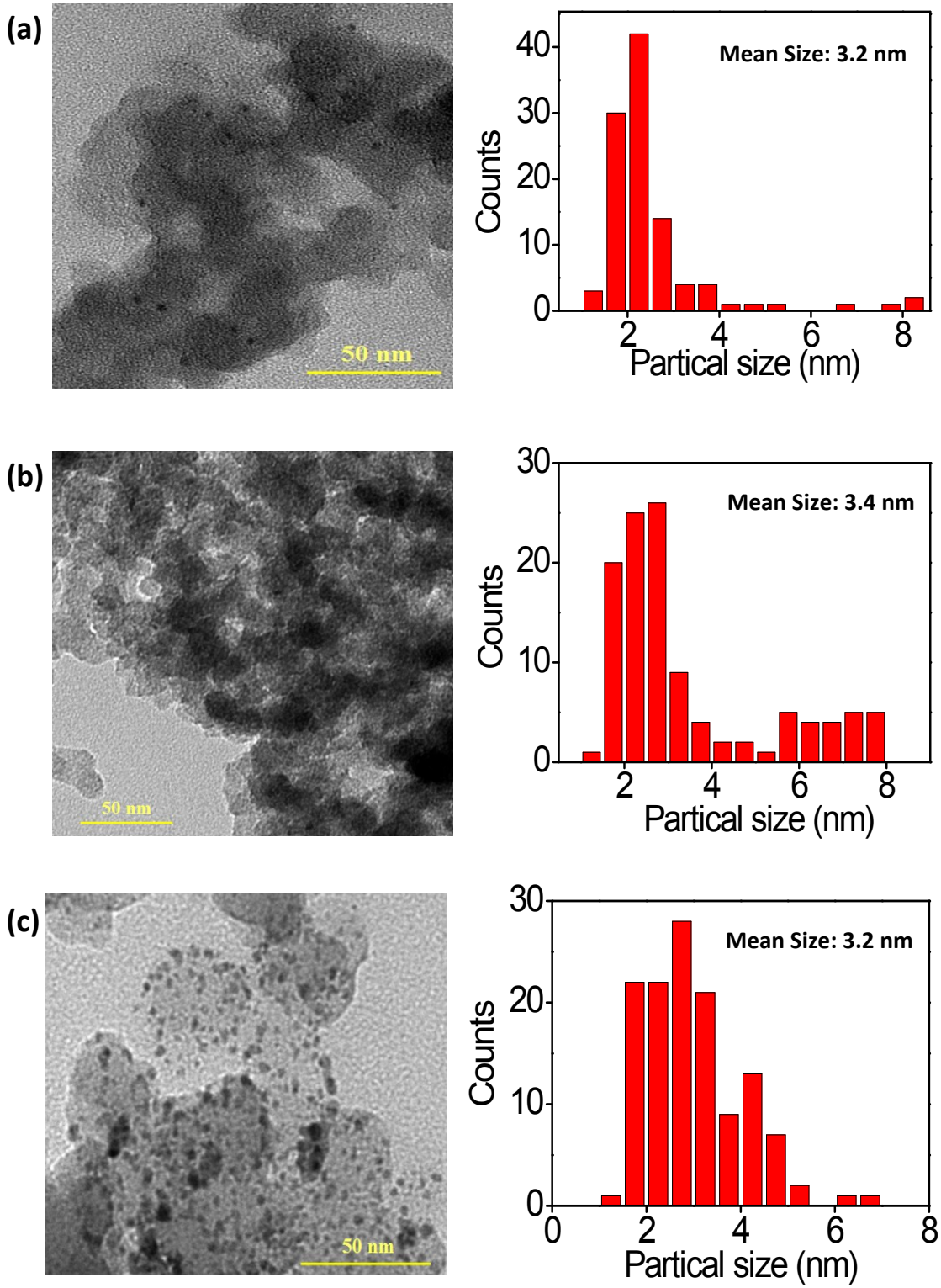


Figure S4. The time-activity profile under different temperatures (conversion below 45%) Below 45% conversion the experimental data fits a zero order plot.

Figure S5. TEM images and particle size distribution of (a) fresh Pd/CN, (b) reused Pd/CN, (c) fresh Pd/Cs and (d) reused Pd/Cs.



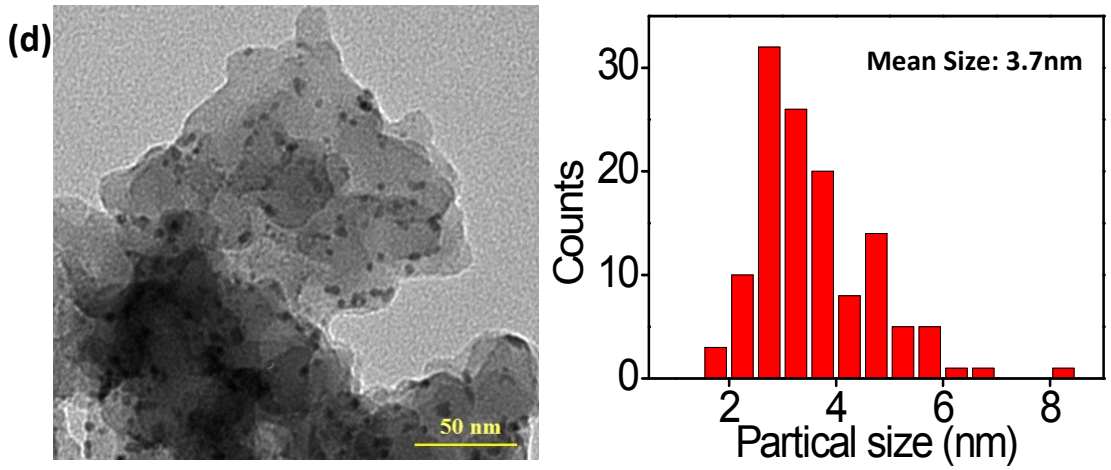


Figure S6. The percentage of dihydrochalcone as a function of reaction time

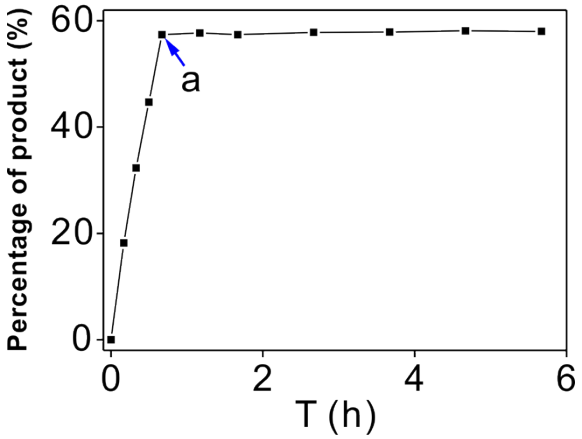


Figure S6. The percentage of dihydrochalcone as a function of reaction time. Reaction conditions: chalcone (0.5 mmol), Pd (0.28 mol% relative to substrate), CH_3CH_2OH (5 mL), temperature (35 ^oC), H_2 (1 bar pressure). Remove the catalyst and get the filtrate at the point of a. Content of the mixture is determined by GC.

As shown in Figure S6, 57.4% conversion of chalcone was achieved within 0.67 h at 35 ^oC with 1 bar hydrogen and the percentage of dihydrochalcone was 57.4% at 0.67 h. Then we removed the catalyst and got the filtrate by centrifugation. Next, the filtrate was introduced into a three-neck flask directly and the reaction was conducted maintaining the identical conditions above. Interestingly, the percentage of product remained static when we prolonged the reaction time to 5.67 h，indicating that the contribution of the leached species could be ignored.

Figure S7. XPS spectra of the fresh and recycled catalyst, Pd/CN

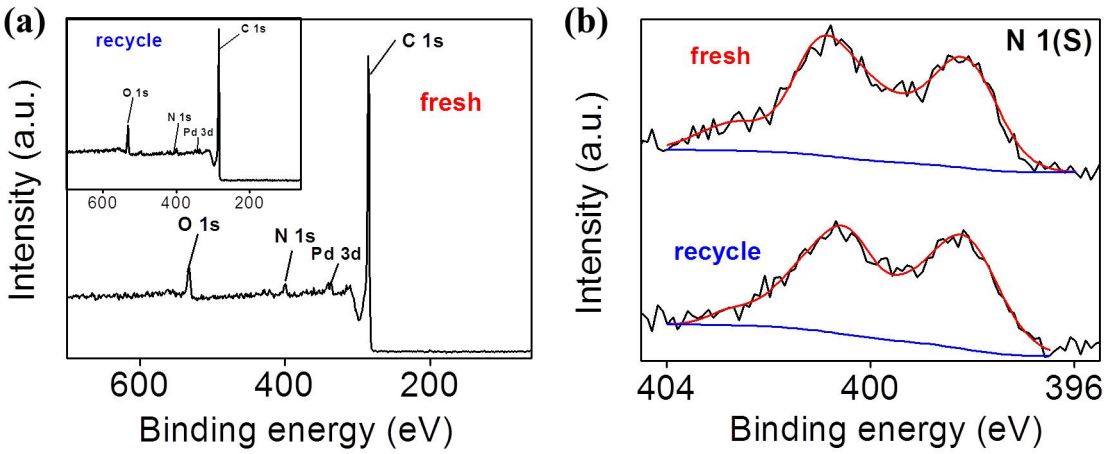


Figure S7. XPS spectra of the fresh and recycled catalyst, Pd/CN: (a) survey spectra; (b) N1s spectra.

The XPS survey spectra of the fresh catalyst shows strong signals from carbon, oxygen, nitrogen and palladium elements, as same as the catalyst after 8 runs (Figure S7a). What is more, the distribution and the shape of N1s spectrum for the recycled catalyst were pretty much the same as the fresh catalyst (Figure S7b). This suggests that the nature and the content of nitrogen species in the surface of the fresh and recycled catalyst are almost the same. The nitrogen functionalities on the surface might act as Lewis base sites and are expected to be more effective in retaining metal nanoparticles. Simultaneously, N-doped carbon material enriches the electron density of the metallic Pd and accelerates the reaction. Taking into account of the above results, a conclusion may be drawn that the nitrogen in the support has a marked influence in the activity and durability of Pd/CN.